Supplementary Table 1. Crystallographic data and refinement statistics.

Structure	S46Y	S46Y, Zn peak	S46Y, Zn remote
Data collection			
Wavelength (Å)	0.9763	1.2815	1.2848
Unit cell parameters			
a,b,c (Å)	47.83, 73.51, 76.12	47.49, 73.13, 75.78	47.65, 73.29, 75.91
α,β,γ (degrees)	$\alpha=\beta=\gamma=90$	$\alpha=\beta=\gamma=90$	$\alpha=\beta=\gamma=90$
Space group	$P22_12_1$	$P22_12_1$	$P22_12_1$
Solvent content (%)	56.64	56.64	56.64
Protein chains in AU	2	2	2
Resolution range (Å)	39.94-1.60	47.79-1.61	47.65-1.61
Highest resolution shell (Å)	1.69-1.60	1.69-1.61	1.70-1.61
Unique reflections	34555 (5013)	35203 (5075)	35198 (5072)
Redundancy	3.5 (3.1)	7.2 (7.3)	7.3 (7.4)
Completeness (%)	96.9 (97.5)	99.9 (100)	99.9 (100)
***R_{merge}**	0.070 (0.439)	0.083 (0.794)	0.064 (0.424)
R_{meas}	0.082 (0.523)	0.104 (0.926)	0.074 (0.493)
Average *I/σ(I)*	9.3 (2.3)	10.9 (2.2)	14.3 (3.7)
Refinement			
R_{work} (%)	15.52		
R_{free} (%)	18.27		
Mean *B* value (Å^2)	29		
B from Wilson plot (Å^2)	16.9		
RMSD bond length (Å)	0.007		
RMSD bond angles (°)	0.859		
No. of amino acid residues	108		
No. of water molecules	303		
No. of metal ions	4		
Ramachandran plot			
Most favored regions (%)	99.55		
Allowed regions (%)	0.45		

Values of the highest resolution shell are given in parentheses.

*$R_{merge} = \Sigma_h\Sigma_l |I_{hl} - \langle I_h\rangle|/\Sigma_h\Sigma_l |\langle I_h\rangle|$